3.9 The ATOM-DISPLAY menu

When DISPLAY is selected in the ATOM-LIST menu (page 26), most of the control buttons are replaced to produce the ATOM-DISPLAY menu. The ATOM-DISPLAY menu has only four control boxes.

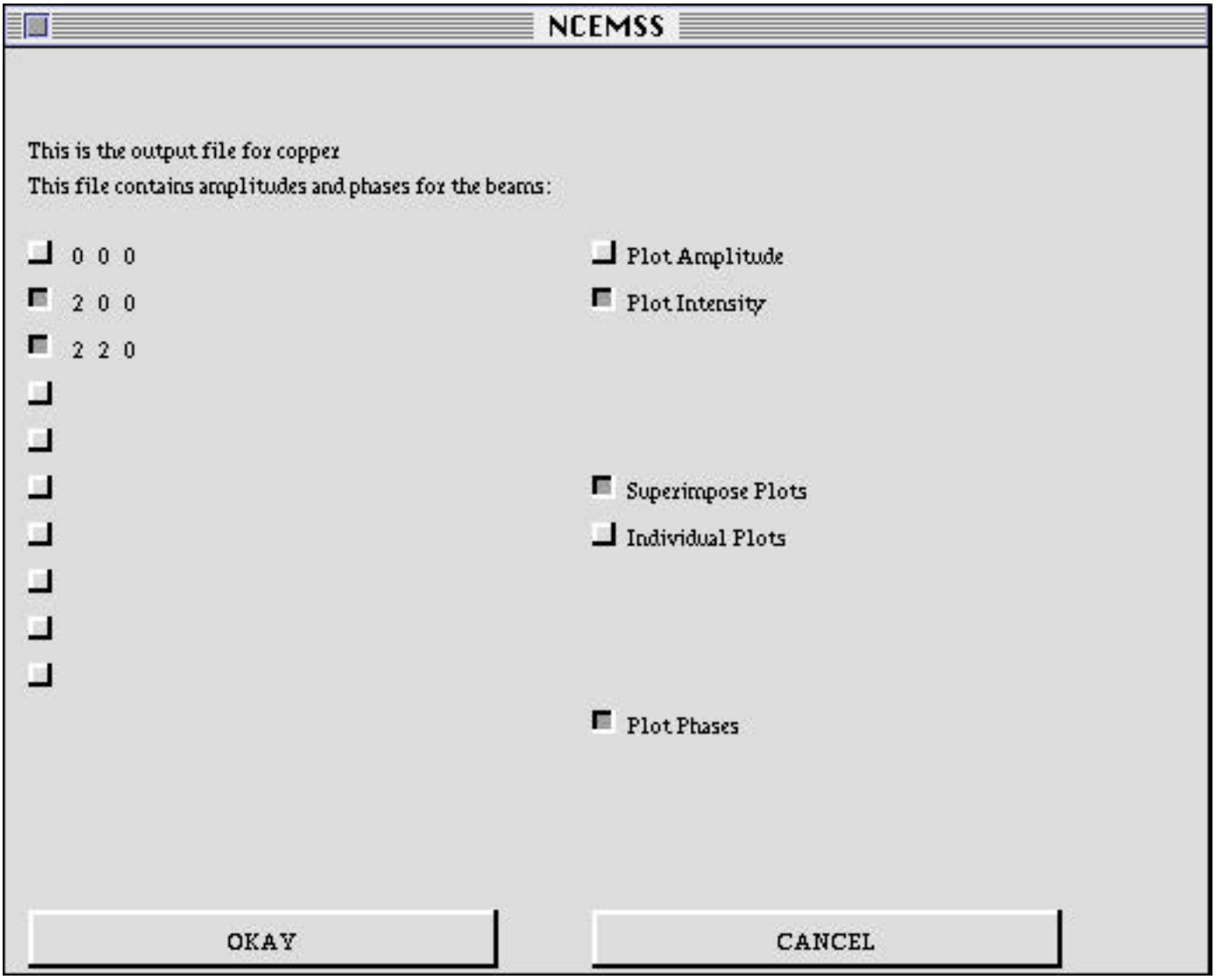
UNIT CELL: Activating this box splits it in two. Selecting either option causes NCEMSS to ask for the viewing direction indices to be input from the keyboard; NCEMSS then draws the unit cell, either with or without perspective (page 32).

NEW UNIT CELL: As for UNIT CELL, but for drawing any new unit cell produced with the BUILD menu (page 28).

3-D ATOM DISPLAY: This control box initiates a three-dimensional atom drawing routine based on a routine written by W.O. Saxton. It can be used to produce publication-quality atom model drawings with a wide range of different lighting conditions. This procedure is not implemented on most versions of NCEMSS, specifically all unix version

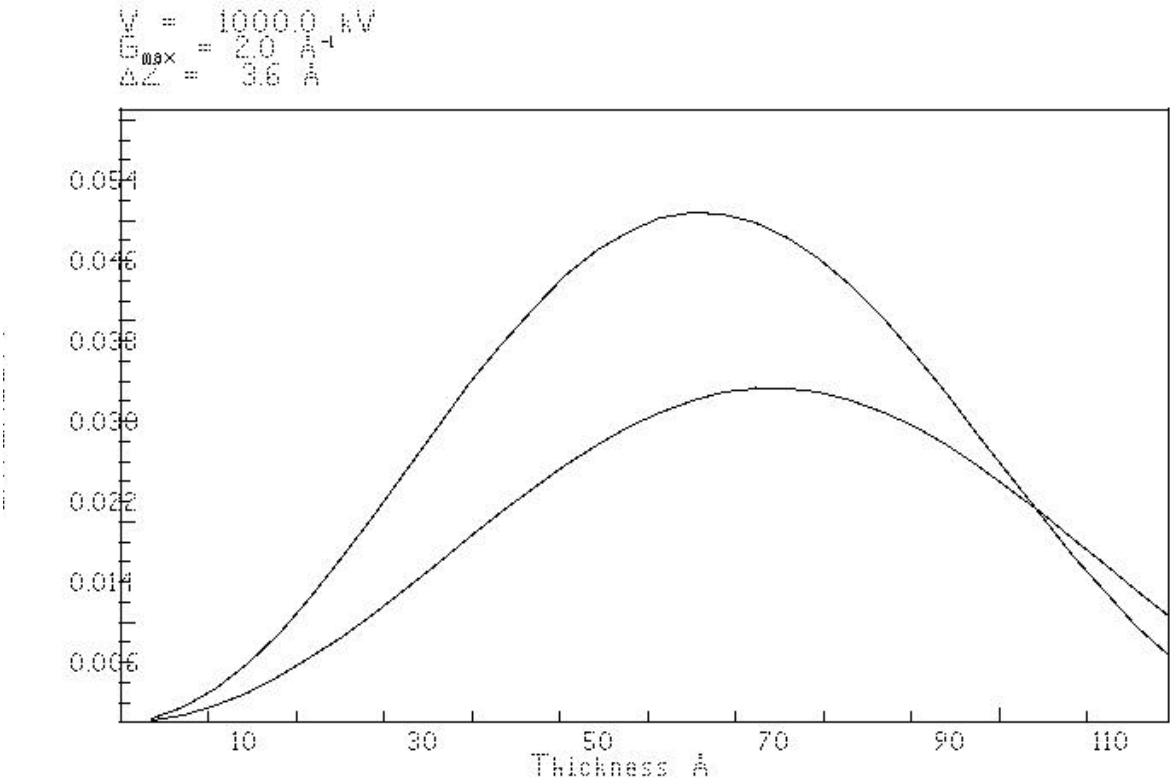
RETURN: Return to previous ATOM-LIST menu.

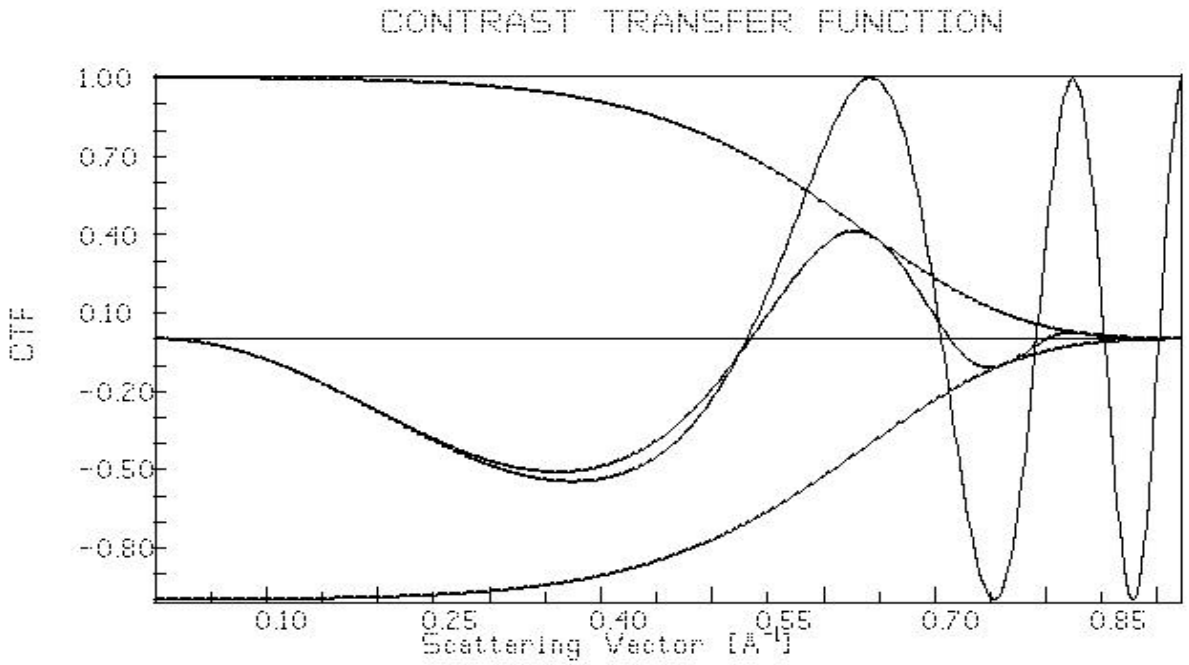
The AMPLIT Menu



3.10 The AMPLIT menu

On activating the AMPLIT control box on the MAIN menu, the user will be presented with a list of the diffracted beams for which the complex amplitudes are currently stored as a function of specimen thickness. NCEMSS will ask the user to select which beams to plot, whether to superimpose the plots, and whether to include phase plots. The plots will be drawn with thickness horizontal and marked in Angstrom units. The various curves can be marked with the appropriate beam indices by using the TEXT option of the SET-UP menu (page 38).

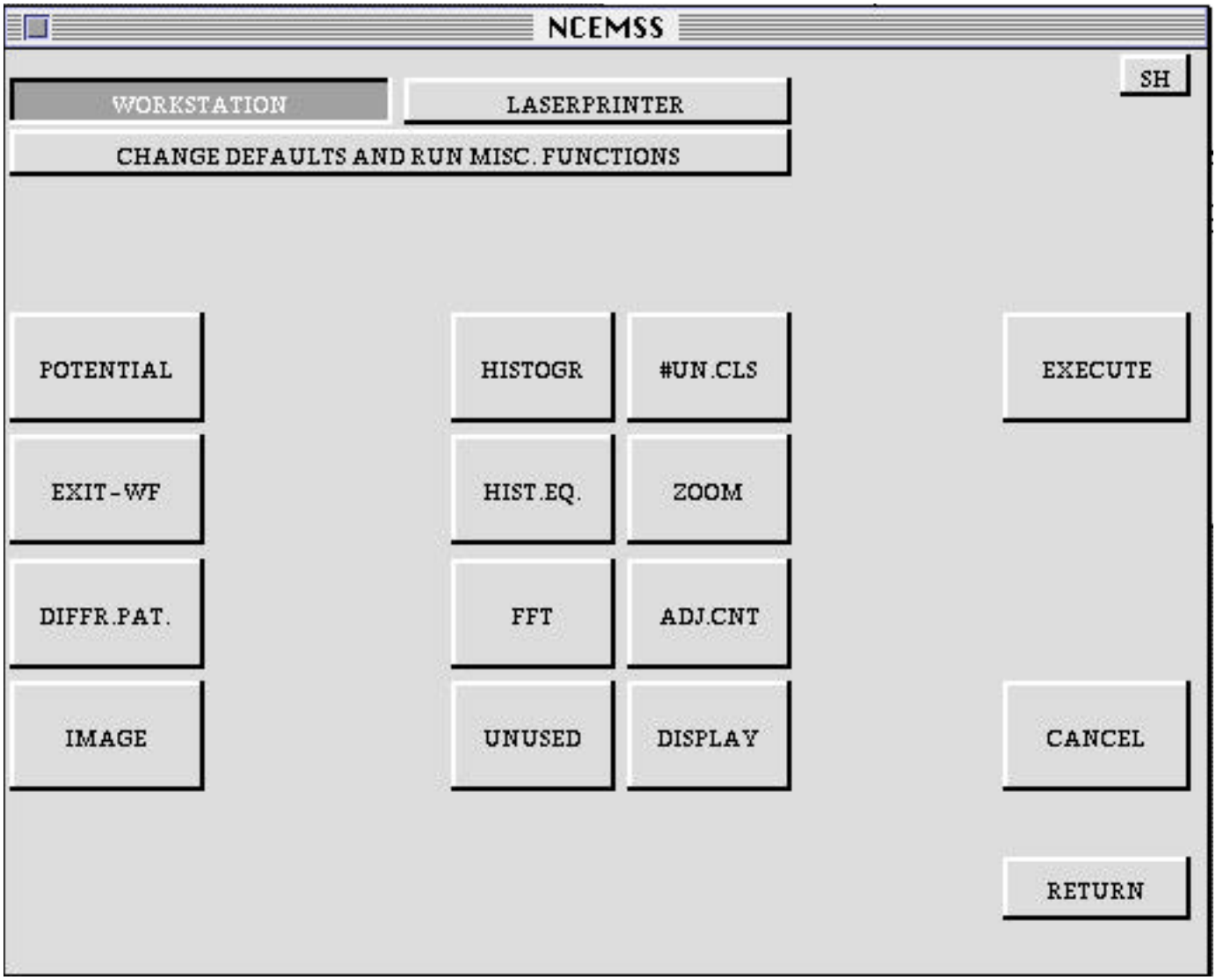



CONTRAST TRANSFER FUNCTION
1.00
0.70
0.40
0.10
-0.20
-0.50
-0.80
CTF
0.10
0.25
0.40
0.55
0.70
0.85
Scattering Vector [A-1]
Accel.Voltage = 1000.0 kV
Spher. Abber. = 2.8 mm
Obj. Lens Def. = -300 A
Delta = 100 A
Div. Angle [Half] = 0.60 mrad

3.11 The CTF plot

The result of activating the CTF control button on the MAIN menu is a plot of the linear-image Contrast Transfer Function. This function is first plotted as the undamped sine part of the complex phase change due to the objective lens spherical aberration and defocus. The damping curves due to the effects of spatial and temporal coherence (incident beam convergence and spread of defocus) are plotted next, then finally the result of imposing the damping on the sine curve. Remember that this curve is only useful for estimating the linear contribution to the image of the diffracted beams exiting a thin crystal (one in which they have suffered only essentially kinematic scattering).

The IMAGE-DISPLAY Menu



3.12 The IMAGE-DISPLAY menu

When DISPLAY is selected in the MAIN or CONTROL menu (page 16), NCEMSS brings up the IMAGE-DISPLAY menu. This menu consists of 21 control buttons. The top three are used to select various options that remain until reset. The left-hand column is used to select the function to be displayed. Other control boxes select the actions to be taken.

WORKSTATION/LASERPRINTER: These two boxes are mutually exclusive and are used to select the output device for the image display.

CHANGE DEFAULTS AND RUN MISC. FUNCTIONS: This control is used to bring up the SET-UP menu (page 40) where various imaging options and defaults may be set.

POTENTIAL: Selecting this input produces a display of the unit cell potential projected in the incident electron beam direction.

EXIT-WF: The electron wavefield at the crystal exit surface may be displayed by selecting this input function.

DIFFR.PAT.: Selects the diffraction pattern for display.

IMAGE: Selects the current image for display.

HISTOGR: Produces a histogram of the intensity values in the function selected from column one.

HIST.EQ.: Stretches the image contrast by performing a histogram equalization operation before display.

ADJ.CNT: Brings up the SET-CONTRAST menu (page 44) for selection of contrast parameters before display.

FFT: Performs a fast Fourier transform on the selected function and squares the result before display. (Performed on the image, FFT produces the image power spectrum or "optical diffractogram").

#UN.CLS: Enables input of the number of unit cells desired in the displayed image.

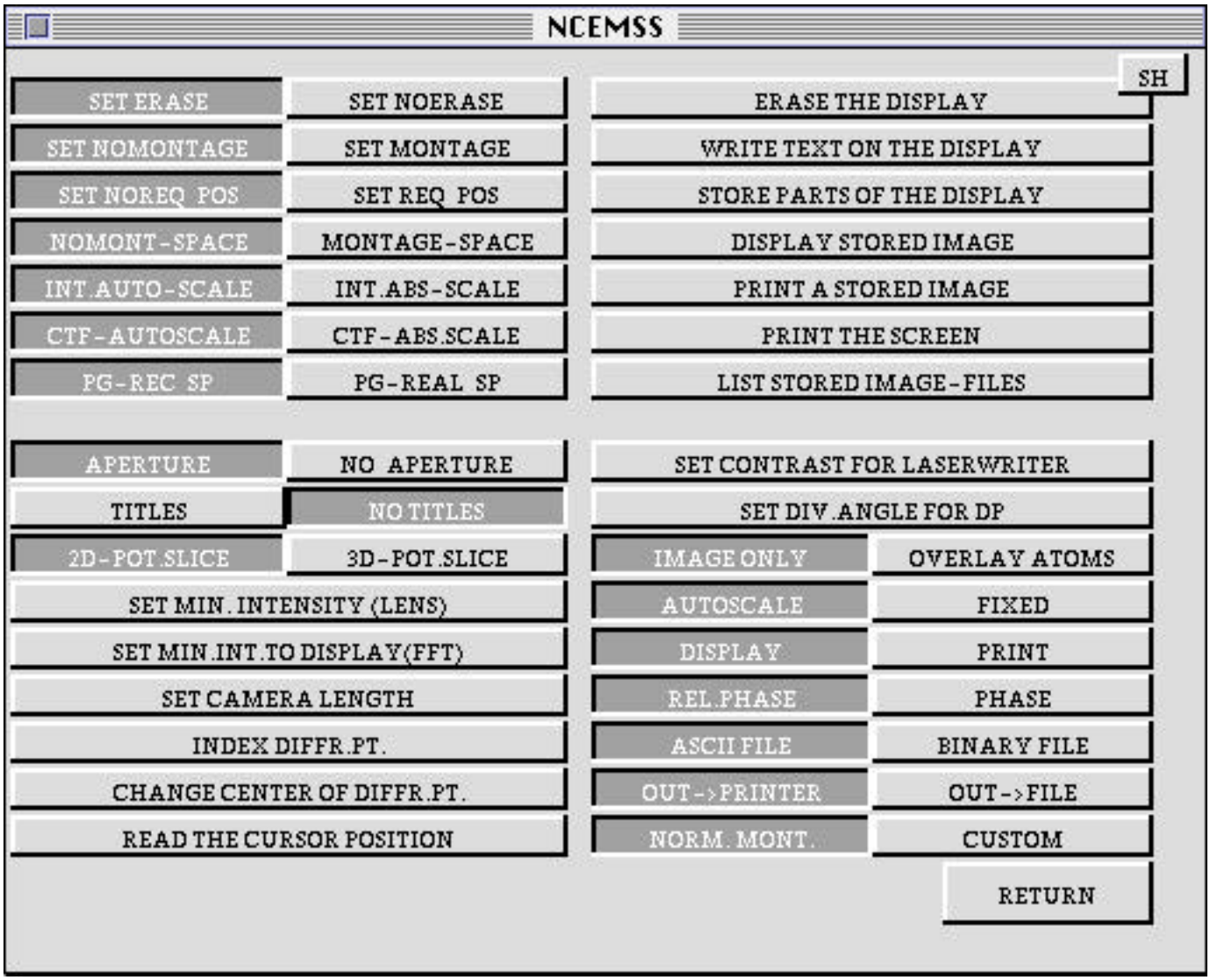
ZOOM: Asks for a factor to use in magnification the image.

DISPLAY: Directs the output to the display device.

EXECUTE: Takes the selected function, applies the selected operations, and outputs the picture.

CANCEL: Cancels the selected options, usually because one was selected by mistake.

The SET-UP Menu



3.13 The SET-UP menu

Opting to change the various defaults by selecting the CHANGE box in the IMAGE-DISPLAY menu (page 38), brings up the SET-UP menu. This menu is used to change the default settings of some "hard" parameters, and to manipulate the image display. The nine two-way switches on the left of the menu are normally set to default to the left-hand setting.

SET ERASE<>NOERASE: When ERASE is set, the display screen will be erased before each new image is displayed (except see MONTAGE).

SET NOMONTAGE<>MONTAGE: When NOMONTAGE is set, only one image will be displayed for each activation of the EXECUTE command from the IMAGE-DISPLAY menu (page 38). When MONTAGE is set, then a full through-thickness and/or through-focus series of images will be displayed at one EXECUTE command (assuming the calculation was carried out for such a series by setting the appropriate parameter values in the PARAMETER menu (page 16)). Note that a MONTAGE will erase the screen before display, regardless of the ERASE setting.

SET NOREQ-POS<>REQ-POS: When NOREQ_POS is set, individual images will be written to the center of the display screen (assuming that NOMONTAGE is set). When REQ_POS is set, the user will be prompted for the coordinates at which the image is to be displayed.

NOMONT-SPACE<>MONTAGE-SPACE: is used to set the desired spacing between the montaged images.

INT.AUTO-SCALE<>INT.ABS-SCALE: To see the most detail in any image, set INT.AUTO-SCALE to display the image with its minimum set to black and its maximum to white. To intercompare images, it is better to use INT.ABS-SCALE to choose the same absolute scale for all the images.

CTF-AUTOSCALE<>CTF-ABS.SCALE: Can be used to scale a CTF plot (page 36) by fixing the maximum g value considered. In AUTOSCALE mode the CTF is drawn to where it approaches zero.

PG-REC SP<>PG-REAL SP: determines whether or not the calculation is done in reciprocal space or in real space. This switch should be set to reciprocal space since the real space calculation is not debugged yet.

APERTURE<>NO-APERTURE: determines whether or not the current objective aperture radius is drawn on a displayed diffraction pattern.

TITLES<>NO TITLES: determines whether titles are written under each displayed image. Notice that MONTAGE will supress titles, but a title for the montaged series may be added using WRITE TEXT.

2D-POT.SLICE<>3D-POT.SLICE: When the number of slices per unit cell exceeds one in the MAIN menu (page 16), NCEMSS will sub-slice the unit cell in one of two ways. When 2D-POT is set, the total potential within the cell will be projected, and a portion assigned to each sub-slice. A more-accurate method is to approximate the upper-layer zones by sub-slicing a three-dimensional potential into the required number of sub-slices. In this way the variation of the specimen structure in the electron beam direction is included in the simulation. Of course, it takes longer in 3-D).

SET MIN. INTENSITY (LENS): sets the minimum diffracted beam intensity that will be considered to pass through the objective lens; this minimum can be set to exclude very low intensity beams from large defect unit cells, and so speed up the image calculation.

SET MIN.INT.TO DISPLAY(FFT): determines down to what intensity diffracted beams will be drawn in a diffraction pattern display.

he SET-UP Menu